

10/536,766

=> file casreact
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FILE CONTENT:1840 - 27 Oct 2007 VOL 147 ISS 19

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*

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L2 133 SEA FILE=CASREACT SSS FUL L1 (568 REACTIONS)
L3 4 SEA FILE=CASREACT L2 AND (ZIRCONIU? OR HAFIU?)

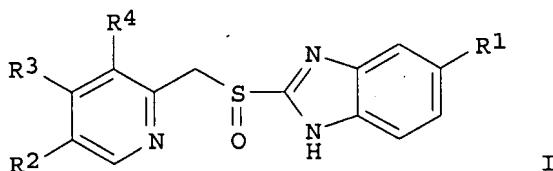
=> d 13 1-4 ibib abs fcrd

L3 ANSWER 1 OF 4 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 147:257772 CASREACT
TITLE: Process for preparation of chiral benzimidazolyl pyridylmethyl sulfoxides from the corresponding sulfides using chiral transition metal complexes and oxidizing agents.
INVENTOR(S): Dubey, Sushil Kumar; Vig, Gaurav; Singh, Anand; Tripathi, Sushil; Paul, Soumendu
PATENT ASSIGNEE(S): Jubilant Organosys Limited, India
SOURCE: PCT Int. Appl., 21pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007088559	A1	20070809	WO 2007-IN35	20070131
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,				

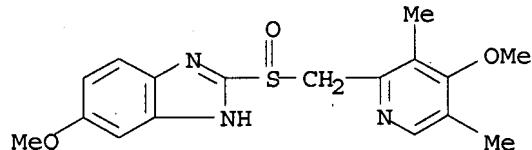
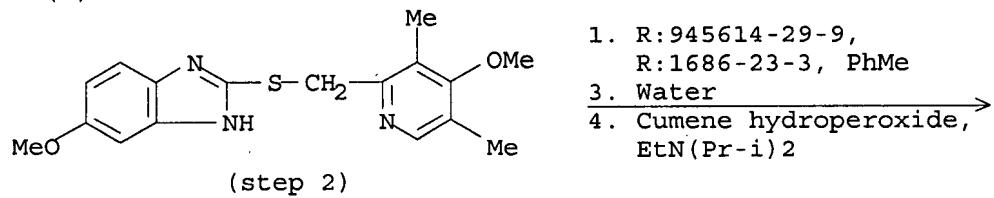
MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
 RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: IN 2006-DE271 20060201
 OTHER SOURCE(S): MARPAT 147:257772
 GI



AB Title compds. (I; R1-R4 = H, alkyl, alkoxy, aryl, aryloxy), were prepared by treatment of the corresponding prochiral sulfides with chiral transition metal complexes and oxidizing agents optionally in presence of an organic solvent, wherein the chiral ligands comprise dicyclohexylidene, diacetonide, or benzylidene derivs. of sugars. Thus, vanadium oxytripropoxide and 1,2,4,5-Di-O-cyclohexylidene-D-fructofuranose were stirred together for 10-15 min in PhMe; 5-methoxy-2-[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]thio]-1H-benzimidazole and H2O were added and the mixture was heated at 50-55° for 1 h; the mixture was cooled to 25-30° followed by addition of diisopropylethylamine and cumene hydroperoxide over 1 h followed by stirring for 45 min. and workup to give 5-methoxy-2-[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole, sodium salt in 75% enantiomeric excess.

RX(1) OF 1



NOTE: alternative preparation shown, stereoselective

CON: STAGE(1) 10 - 15 minutes, room temperature

STAGE(2) room temperature -> 55 deg C

STAGE(3) 1 hour, 50 - 55 deg C; 55 deg C -> 30 deg C

STAGE(4) 1 hour, 25 - 30 deg C; 45 minutes, 25 - 30 deg C

REFERENCE COUNT:

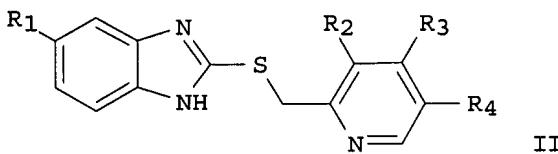
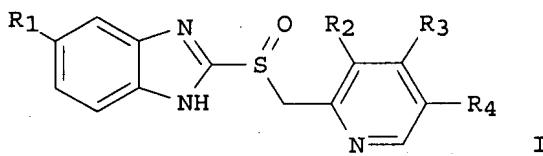
4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 4 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 144:390922 CASREACT
 TITLE: Stereoselective oxidation processes for the preparation of chiral substituted sulfoxides from the racemic sulfides
 INVENTOR(S): Kumar, Neela Praveen; Khanna, Mahavir Singh; Prasad, Mohan; Kumar, Yatendra
 PATENT ASSIGNEE(S): Ranbaxy Laboratories Limited, India
 SOURCE: PCT Int. Appl., 23 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006040635	A1	20060420	WO 2005-IB2946	20051004
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1802584	A1	20070704	EP 2005-790107	20051004
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
IN 2007DN03340	A	20070831	IN 2007-DN3340	20070503
PRIORITY APPLN. INFO.:			IN 2004-DE1957	20041011
			WO 2005-IB2946	20051004

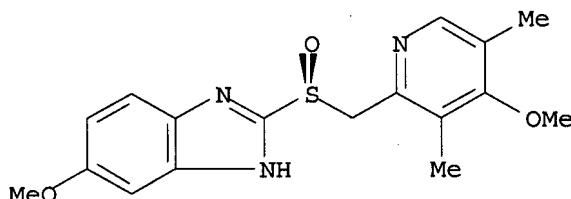
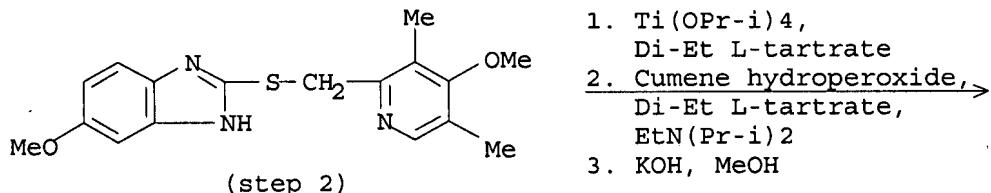
OTHER SOURCE(S): MARPAT 144:390922
 GI



AB An enantioselective catalytic oxidation process for the preparation of an optically active enantiomer or an enantiomerically enriched form of a substituted pyridylmethylsulfinylbenzimidazole [I; R1-R4 = H, C1-4 (un)branched alkyl, C1-4 (un)branched alkoxy, aryl, aryloxy], or its pharmaceutically acceptable salts (e.g., esomeprazole potassium), comprises oxidizing a prochiral sulfide (II; e.g., omeprazole sulfide) in

the presence of a chiral transition metal complex [e.g., titanium isopropoxide and L-(+)-diethyl tartrate] and a base (e.g., diisopropylethylamine) in the absence of an organic solvent with an oxidant (e.g., cumene hydroperoxide) followed by an optional salification (e.g., potassium hydroxide).

RX(1) OF 3



K

NOTE: optimization study, stereoselective

CON: STAGE(1) room temperature \rightarrow 50 deg C; 1.5 hours; 25 - 30 deg C

STAGE(2) 25 - 30 deg C; 3 hours, 25 - 30 deg C

STAGE(3) 25 - 35 deg C; 15 - 16 hours, 25 - 35 deg C

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 144:51582 CASREACT

TITLE: Process for the preparation of pyridin-2-ylmethylsulfinyl-1H-benzimidazoles via oxidation of the corresponding sulfides in the presence of zirconium or hafnium complexes.

INVENTOR(S): Kohl, Bernhard; Mueller, Bernd; Weingart, Ralf Steffen

PATENT ASSIGNEE(S): Altana Pharma AG, Germany

SOURCE: PCT Int. Appl., 15 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005118569	A1	20051215	WO 2005-EP52471	20050531
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,				

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2005250175 A1 20051215 AU 2005-250175 20050531

CA 2568652 A1 20051215 CA 2005-2568652 20050531

EP 1758889 A1 20070307 EP 2005-752651 20050531

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU

CN 1960987 A 20070509 CN 2005-80017526 20050531

US 2007225500 A1 20070927 US 2006-597373 20061122

KR 2007031945 A 20070320 KR 2006-726831 20061220

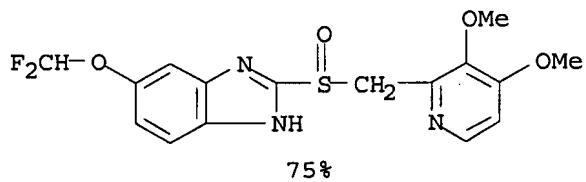
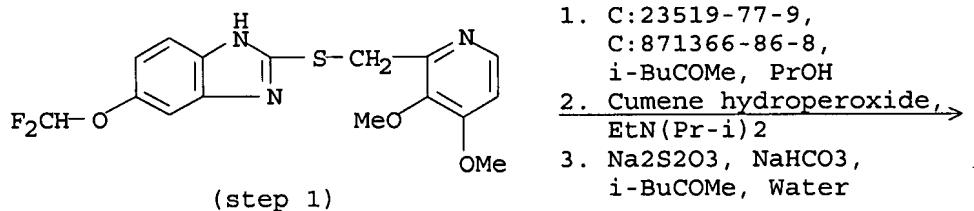
IN 2006MN01589 A 20070615 IN 2006-MN1589 20061220

NO 2006006003 A 20061222 NO 2006-6003 20061222

PRIORITY APPLN. INFO.: EP 2004-102467 20040602
WO 2005-EP52471 20050531

AB A process for preparing mixts. of enantiomers of proton pump inhibitors (PPIs) having a sulfinyl structure comprises oxidation of the corresponding sulfides in the presence of a mixture of enantiomers of chiral zirconium or hafnium complexes. Thus, 5-difluoromethoxy-2-[(3,4-dimethoxy-2-pyridinyl)methylthio]-1H-benzimidazole was heated with DL-tartaric acid bis(N-pyrrolidinamide) and zirconium tetra-n-propoxide in Me iso-Bu ketone at 40° for 1 h followed by addition of diisopropylethylamine and slow addition of cumene hydroperoxide to give 75% 5-difluoromethoxy-2-[(3,4-dimethoxy-2-pyridinyl)methylsulfinyl]-1H-benzimidazole.

RX(1) OF 1



NOTE: optimization study

CON: STAGE(1) 1 hour, 40 deg C; 40 deg C -> room temperature

STAGE(2) room temperature; 5 - 24 hours, room temperature

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 4 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:54346 CASREACT

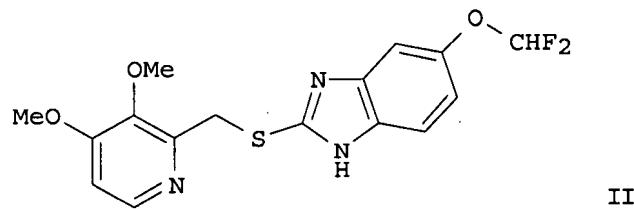
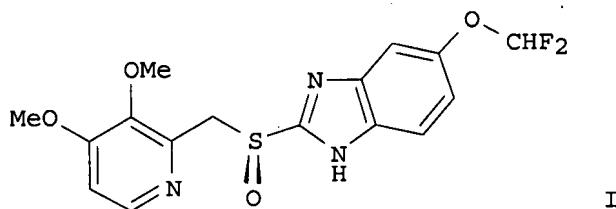
TITLE: A process for preparing (S)-pantoprazole via

stereoselective oxidation of pyridinylmethylsulfinylbenzimidazole derivative in the presence of L-tartaric acid derivative and chiral zirconium or hafnium catalyst

INVENTOR(S): Kohl, Bernhard; Mueller, Bernd; Weingart, Ralf Steffen
 PATENT ASSIGNEE(S): Altana Pharma Ag, Germany
 SOURCE: PCT Int. Appl., 14 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004052881	A2	20040624	WO 2003-EP13604	20031203
WO 2004052881	A3	20041104		
W: AE, AL, AU, BA, BR, CA, CN, CO, DZ, EC, EG, GE, HR, ID, IL, IN, IS, JP, KR, LT, LV, MA, MK, MX, NO, NZ, PH, PL, SG, TN, UA, US, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2507889	A1	20040624	CA 2003-2507889	20031203
AU 2003293749	A1	20040630	AU 2003-293749	20031203
EP 1575941	A2	20050921	EP 2003-789113	20031203
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003016702	A	20051018	BR 2003-16702	20031203
CN 1717402	A	20060104	CN 2003-80104409	20031203
JP 2006514985	T	20060518	JP 2005-502309	20031203
MX 2005PA05761	A	20050816	MX 2005-PA5761	20050530
IN 2005MN00673	A	20051021	IN 2005-MN673	20050627
US 2006167262	A1	20060727	US 2005-536891	20051125
PRIORITY APPLN. INFO.:			EP 2002-27274	20021206
			DE 2003-10340254	20030829
			WO 2003-EP13604	20031203

GI

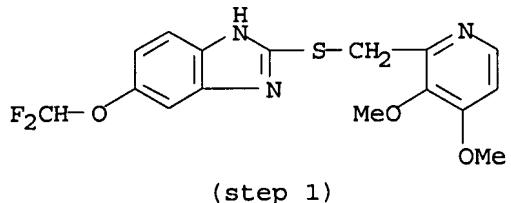


AB The invention relates to a novel process for preparing (S)-pantoprazole (I) via stereoselective oxidation of pyridinylmethylsulfinylbenzimidazole derivative

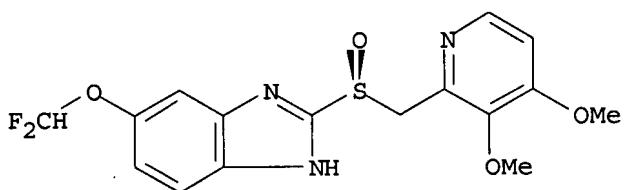
in the presence of L-tartaric acid derivative and chiral zirconium or hafnium catalyst. For instance, the title compound I, useful as proton pump inhibitor, was prepared from thiobenzimidazole derivative II in the presence of L-tartaric acid amide via Zr(IV) isopropoxide catalyzed oxidation

by cumene hydroperoxide with a yield of 80% (optical purity was >98%, example 3).

RX(1) OF 1



1. C:63126-10-3,
i-BuCOMe
2. C:23519-77-9,
Me2CHOH
3. EtN(Pr-i)2,
Cumene hydroperoxide,
S:98-82-8
4. NaHCO3, Na2S2O3,
Me2CHOH, Water



NOTE: optimization study, optimized on catalyst, stereoselective

CON: STAGE(1) 40 - 45 deg C

STAGE(2) 40 - 45 deg C; 1 hour; 30 deg C

STAGE(3) 20 hours, 30 deg C

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